SESSION Q14: DMP: ORDER-DISORDER PHENOMENA IN SEMICONDUCTORS I
Friday morning, 26 March 1993; Room 210 at 8:OO; E. Jones. presiding

Invited Papers

8:00

Q14 1 Spontaneous Ordering in Semiconductor Alloys.'

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Vapor-phase (MOCVD, MBE, ALE) growth of many $A_{1-x}B_xC$ semiconductor alloys results in spontaneous long-range order, most often in the form of monolayer-alternation $(AC)_1/(BC)_1$ superlattices along the (111) direction (the "CuPt" structure). At the same time, it is known theoretically that: (i) the lowest energy state of ***bulk*** alloys is phase-separation into AC + BC, and that (ii) the lowest energy state of ***epitaxial*** alloys is the ABC, chalcopyrite structure. A combination of first-principles total energy calculations and lattice-gas thermodynamic models [l] clarifies that: (i) phase-separation is inhibited by the epitaxial coherence with the substrate, (ii) the chalcopyrite structure is surface-unstable relative to the CuPt structure. and (iii) dimerization, bucking and tilting of surface cations stabilizes even at T~900K a special variant ("CuPt-B") of the CuPt structure. Spontaneous ordering changes profoundly the band structure of the alloy **[2],** leading to (a) bandgap reduction, and (b) splitting of the degeneracy of the valence band maximum. These reflect L-point zone folding and crystal-field effects, respectively. I will discuss the electronic structure of random, ordered and partially-ordered alloys, demonstrating new opportunities for alloy bandgap engineering at fixed composition, including the possibility [3] of attaining far-IR bandgaps of ***ordered*** III-Vs.

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+ In collaboration with J.E. Bernard, S. Froyen, R. Osorio and S.-H. Wei.
[l] Froyen. zunger, Phys. Rev. Lett. **66, 2132** (1991); Bernard, Froyen. Zunger, Phys. rev. B 44, 11178 (1991); Osorio, Bernard. Froyen and zunger, **ibid 45,** 11173 (1992)
[2] Wei and Zunger, Appl. Phys. Lett. 56, 662 (1990); Laks, Wei and Zunger, Phys. Rev. Lett, (December 24, 1992)
[3] Wei and Zunger, Appl. Phys. Lett 58, **2684** (1991).